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EVOLUTION OF DEFLAGRATION IN A COLD COMBUSTIBLE SUBJECTED TO A --ETC(U)  
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EVOLUTION OF DEFLAGRATION IN A COLD  
COMBUSTIBLE SUBJECTED TO A UNIFORM  
ENERGY FLUX

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MATHEMATICS RESEARCH CENTER

EVOLUTION OF DEFLAGRATION IN A COLD COMBUSTIBLE  
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A. K. Kapila\*

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ABSTRACT

↓  
The title problem is treated in the limit of large activation energy. It is shown that the evolutionary process takes place in a series of distinct stages, and the spatial and temporal structure of each stage is described. It is found that subsequent to thermal runaway, the behavior of the system resembles that of self-induced combustion, except that the thermal explosion is now confined to a thin surface layer. → to page 4

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#### SIGNIFICANCE AND EXPLANATION

Burning of an initially cold combustible material is studied. It is assumed that combustion is initiated by heating the surface of the material. This will result in a chemical reaction first occurring at the surface, and then spreading through the material in the form of a flame or deflagration wave. Asymptotic methods are used to study the transient process leading to the establishment of the flame. Attention is confined to solid combustibles, but it is envisaged that the techniques developed here will aid in the eventual understanding of the evolution of gaseous combustion.

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# EVOLUTION OF DEFLAGRATION IN A COLD COMBUSTIBLE

## SUBJECTED TO A UNIFORM ENERGY FLUX

A. K. Kapila\*

### 1. INTRODUCTION

Consider a combustible material confined to a container and capable of undergoing an exothermic chemical reaction of the Arrhenius type. There are essentially two modes by which burning can be initiated in this system: either through self-induced heating (thermal explosion) or by an external stimulus (ignition). In the first mode the initial temperature of the material is high enough so that a significant amount of chemical heat release begins to occur immediately throughout the system. If heat loss is not overpowering the temperature will rise, but seldom uniformly in space. The fastest rise usually occurs at one or more discrete sites where hot spots form and eventually combustion waves originate.

A detailed mathematical treatment of the dynamics of self-induced combustion for a diffusional-thermal model has recently been given by Kapila [1]. A symmetric geometry is chosen so as to lead to the development of precisely one hot spot, and the spatial and temporal structures of the various phases of the evolutionary process are described. It is shown that while the birth of the hot spot is a rather slow phenomenon, its growth and transition into a deflagrating wave are extremely rapid events indeed. A partial development along the same lines, undertaken independently and including extensions to several geometries, is due to Kasso and Poland [2-4].

The above treatments have all been asymptotic, based upon the limit of large activation energy. This limit, although in implicit use since the early work of Zeldovich and Frank-Kamenetskii (see, for example, [5] and [6]), was suggested as the basis for a rational asymptotic theory only recently by Williams [7]. Since then it has been applied

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successfully to a wide variety of problems in combustion theory, and in fact has inspired a forthcoming monograph on the subject by Buckmaster and Ludford [8]. In the present context, Kasso's extensive investigations (see [9] and the references contained therein) of the spatially uniform thermal explosion deserve special mention.

In the ignition mode the initial temperature of the combustible is so low that it is practically inert, and will not burn if left alone. Energy transfer from an external source is therefore needed to activate the chemistry. This raises a natural question: how long should the external stimulus be maintained before the material is sufficiently excited to develop self-sustained combustion? Attempts to treat this question embody the classical theory of ignition. For solid combustibles the status of the theory, and the pertinent literature as of 1970, are contained in the review article by Merzhanov and Averson [10]. From a theoretical standpoint, two problems appear to have received the most attention. These treat a homogeneous, semi-infinite reactive solid, heated either by applying a constant energy flux at the surface or by raising and subsequently maintaining the surface temperature. The nonlinear parabolic differential equations governing the problems have either been solved numerically or by a variety of approximating techniques [10]. They all have one common feature: ignition is deemed to have occurred when the solution is perceived to have departed significantly from the chemically inert solution for the same configuration.

The large activation-energy limit has played a clarifying role in ignition theory as well. Thus, most past approximations were rendered obsolete by the recent asymptotic studies of Liñán and Williams [11, 12]. Their work has two important features. First, the onset of ignition is defined by a mathematically precise criterion based upon "thermal runaway". In other words, the solution is sought as a small deviation from the corresponding inert solution, and the instant of ignition is defined to be the one at which the perturbation develops a mathematical singularity. Second, explicit asymptotic expressions are given for the ignition delay period. The results are found to be in close agreement with numerical values available in the literature.

While the above work answers one question satisfactorily, it raises another, namely, what is the post-ignition transient that culminates in the development of a deflagration wave? A description of the transient falls outside the scope of ignition theory, since large departures from inert heating will be involved. The singularity of Linán and Williams' quasi-steady solution does provide a clue, however; it suggests that unsteady effects will have to be reinstated for further development of the solution.

This paper aims at describing the entire sequence of events, subsequent to ignition, for the case of the constant surface-flux stimulus. We shall find that the situation is quite akin to that for the self-induced combustion mode discussed in '1', except that the thermal explosion is now confined to a thin surface layer. The analysis again draws upon large activation-energy asymptotics, and a solution uniformly valid in space and time is sought. The problem corresponding to a step increase in surface temperature will be the subject of another paper.

On physical grounds it is quite clear that for a solid reactant the ultimate state will be one of nearly steady deflagration if heat loss is absent. For a gaseous mixture the situation is not so obvious. Depending upon the strength of the reaction and its coupling with the gas dynamics, the final state may well be a detonation. It is expected that the techniques developed here will aid in the eventual understanding of the evolution of combustion in confined gases.



## 2. MATHEMATICAL FORMULATION.

Consider a combustible material occupying the right-half space  $x' > 0$  and capable of undergoing a first-order, one-step Arrhenius-type chemical reaction. (Primes indicate dimensional quantities.) We envisage a diffusional-thermal model in which the material is assumed to have constant physical properties (density  $\rho'$ , thermal conductivity  $k'$ , material diffusivity  $D'$  for the reactant species, and specific heat  $c'$ ). Initially the temperature is  $\theta'_0$  and the fuel mass fraction  $Y'_0$ . Commencing at time  $t' = 0$ , a constant heat flux  $q'$  is applied at the surface. The equations governing the thermo-chemical behavior of the material are

$$\begin{aligned}\rho'c'\theta'_t &= k'\theta'_{x'x'} + Q'A'Y'\exp(-E'/R'\theta') , \\ \rho'Y'_t &= \rho'D'Y'_{x'x'} - A'Y'\exp(-E'/R'\theta') , \\ k'\theta'_{x'}(0,t') &= -q' , \quad \theta'(\infty,t') = \theta'_0 ; \quad Y'_{x'}(0,t') = 0 , \quad Y'(\infty,t') = 1 , \\ \theta'(x',0) &= \theta'_0 , \quad Y'(x',0) = Y'_0 .\end{aligned}$$

Here  $Q', E', A'$  and  $R'$  are, respectively, the heat of reaction, the activation energy, the pre-exponential factor and the gas constant. On selecting  $\theta'_0, Y'_0, k'\theta'_0/q'$  and  $\rho'c'k'\theta'^2_0/q'^2$  to be the units of temperature, mass fraction, length and time respectively, the above system reduces to the following dimensionless form:

$$\theta_t = \theta_{xx} + AY \exp(-E/\theta) , \quad (2.1a)$$

$$Y_t = L^{-1}Y_{xx} - (A/B)Y \exp(-E/\theta) , \quad (2.1b)$$

$$\theta_x(0,t) = -1 , \quad \theta(\infty,t) = 1 , \quad (2.2a)$$

$$Y_x(0,t) = 0 , \quad Y(\infty,t) = 1 , \quad (2.2b)$$

$$\theta(x,0) = 1 , \quad (2.3a)$$

$$y(x,0) = 1 . \quad (2.3b)$$

The nondimensional parameters appearing above are

$$A = (Q'A'Y'_0k'\theta'_0/q'^2) , \quad \text{the Damkohler number,}$$

$$B = (Q'Y'_0)/(c'\theta'_0) , \quad \text{the heat-release parameter,}$$

$$L = k'/( \rho'c'D' ) , \quad \text{the Lewis number, and}$$

$$E = E'/(R'\theta'_0) , \quad \text{the activation energy.}$$

The mathematical model considered above is quite adequate for an approximate description of solid combustion (but not for gaseous reactants, since material deformation has been ignored) and becomes still more realistic by taking  $L = \infty$ , because diffusion of the solid reactant relative to that of heat is negligible. We shall, however, present the analytical details only for  $L = 1$ ; the special symmetry of the equations then renders the mathematics particularly simple without compromising the essential physics. This was verified by actual computations for  $L = \infty$ , and it was found that the asymptotics must then be taken to higher orders to capture the equivalent results. A discussion of significant departures from the  $L = 1$  case is given in the last section.

Although, as pointed out above, the model under consideration is deficient as a tool for studying the evolution of gaseous combustion, it has provided satisfactory descriptions of several other aspects of gaseous flames. See, for example, accounts of cellular flames [13] and of flames in accelerating environments [14]; also see [15] for a rational derivation of the model from the equations of aerothermochemistry.

Typical values of  $A, B$  and  $E$  are  $10^{15}$ , 2 and 25, respectively (see, for example, Bradley [16]). It is particularly realistic, therefore, to attempt an asymptotic analysis in the limit  $E \rightarrow \infty$ , taking  $B$  to be an  $O(1)$  parameter. The largeness of  $A$  is accounted for by setting

$$A = \bar{A} \exp(E/\theta_c) \quad (2.4)$$

where  $\bar{A}$  is assumed to be at most algebraic in  $E$  for large  $E$ , and will be assigned during the course of the analysis. Thus (2.4) defines  $\theta_c$ , which is assumed to be  $O(1)$ . Also, we let

$$1 < \theta_c < 1 + B. \quad (2.5)$$

The lower limit ensures that combustion is not instantaneous, while the upper limit, as we shall see, allows a self-sustained deflagration wave to propagate into the cold material.

For unit Lewis number, equations (2.1-2.3) show that

$$\theta + BY = \theta_I + B, \quad (2.6)$$

where  $\theta_I$ , the inert temperature, is the solution of (2.1a), (2.2a) and (2.3a) for  $A = 0$ , and is given by

$$\theta_I = 1 + 2(t/\pi)^{1/2} \exp[-x^2/(4t)] - x \operatorname{erfc}[x/(2\sqrt{t})] . \quad (2.7)$$

The result (2.6) effectively eliminates  $Y$  from explicit consideration as a dependent variable. Following Liñán and Williams [10] we recast the  $\theta$ -problem in terms of  $z$ , where

$$z = \theta - \theta_I \quad (2.8)$$

is the departure of  $\theta$  from the inert  $\theta_I$ . Equations (2.4), (2.6) and (2.8) then lead to the reduced system

$$\phi_t = \phi_{xx} + (\bar{A}/B)(R - \phi) \exp[(\theta_C^2/\epsilon)\{\theta_C^{-1} - (\theta_I + \phi^{-1})\}] , \quad (2.9)$$

$$\phi_x(0,t) = \phi(\infty,t) = 0 , \quad (2.10)$$

$$\phi(x,0) = 0 , \quad (2.11)$$

where

$$\epsilon = \theta_C^2/F . \quad (2.12)$$

Our aim is to develop an asymptotic solution, uniformly valid in  $x$  and  $t$ , as  $\epsilon \rightarrow 0$ . The solution will be seen to evolve in several stages, each characterized by a distinct time scale. The longest of these is the inert stage, of  $O(1)$  extent on the time scale  $t$  and characterized by essentially zero chemical activity. A short transition period of  $O(\epsilon)$  duration follows, in which a weak chemical reaction develops in a thin surface layer, eventually leading to thermal runaway. The reaction intensifies during the ignition state,  $O(\epsilon^2)$  long in  $t$ , and a hot spot appears at the surface. The hot spot shrinks and strengthens in an exponentially brief explosion period. A still shorter detachment stage follows, in which the hot spot leaves the surface and begins its advance into the interior. Finally, a well-defined deflagration wave, traveling with practically uniform speed, is established during the slightly longer propagation stage. Thus, in physical terms, the transient beyond the transition stage is similar to that in self-induced combustion, except that the thermal explosion is now confined to a narrow surface layer. We shall take advantage of this similarity to omit details whenever possible, referring the reader to [1] instead. In the interest of clarity, however, some repetition has been unavoidable.

A schematic view of the transient appears in Figure 1.

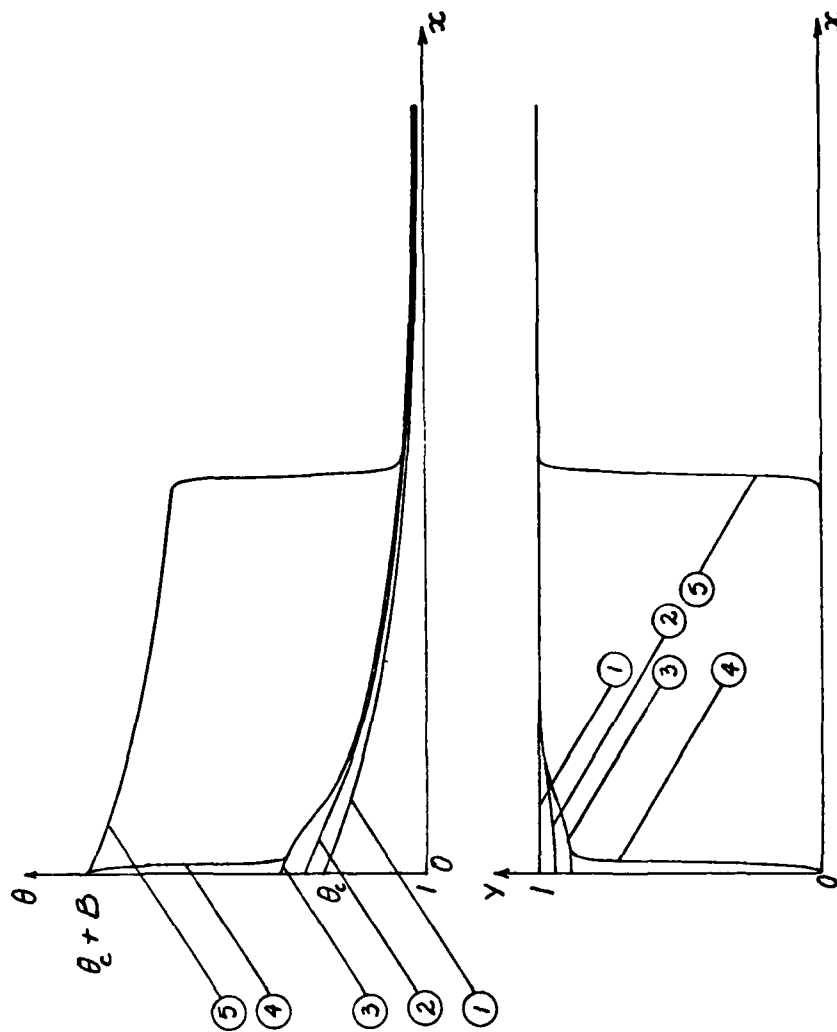


Figure 1. A schematic of the temperature ( $\theta$ ) and concentration ( $\gamma$ ) profiles during the transient. (1): end of inert stage, (2): end of transition stage, (3): end of ignition stage, (4): end of explosion stage, and (5): during propagation stage.

### 3. INERT AND TRANSITION STAGES

The first two stages were treated in detail by Liñán and Williams [11]. In order to continue the solution further it is helpful to briefly reconstruct, and slightly amplify, their analysis.

For small  $t$ ,  $\theta = \theta_I + \phi < \theta_c$ , so that the reaction term in (2.9) is exponentially small. Therefore, the solution to (2.9-2.11) is inert, i.e.

$$\phi = 0 + \text{est}, \quad (3.1)$$

where est stands for exponentially small terms. Correspondingly, (2.6) shows that

$$Y = 1 + \text{est},$$

i.e., reactant consumption has been negligible. This solution becomes void and gives way to the transition stage as soon as the chemical term comes into play in (2.9). This will occur first at the surface (where temperature is at its maximum) at time  $t_c$  such that

$$\theta_I(0, t_c) = \theta_c, \text{ i.e. from (2.7),}$$

$$t_c = \pi(\theta_c - 1)^2/4. \quad (3.2)$$

The argument of the exponential in (2.9) indicates that for  $\epsilon \rightarrow 0$ , chemical activity will be confined to the region where  $\theta_I + \phi - \theta_c = O(\epsilon)$ , i.e. to the thin surface zone  $R_2$  (see Figure 2) where the appropriate independent variables are  $\xi$  and  $\tau$ , defined by

$$x = \epsilon\xi, \quad t = t_c + \epsilon\tau; \quad \xi > 0, \quad \tau > -\infty.$$

Equation (2.9) then reads

$$\epsilon\phi_\tau = \phi_{\xi\xi} + \epsilon^{3/2}(A_0/R)(B-\phi)\exp[\theta_c^2/\epsilon]\{\theta_c^{-1} - (\theta_c + \phi - \epsilon\xi + \epsilon\tau/\sqrt{\pi t_c} + o(\epsilon))^{-1}\}, \quad (3.3)$$

where we have anticipated that

$$\bar{A} = \epsilon^{-1/2}A_0 \quad (3.4)$$

and the expression (2.7) for  $\theta_I$  has been expanded in terms of  $\xi$  and  $\tau$ . The  $O(1)$  constant  $A_0$  will be assigned shortly. We note that to leading order, equation (3.3) is steady. With  $\phi$  expanded as

$$\phi = \epsilon\phi_0(\xi, \tau) + \epsilon^{3/2}\phi_1(\xi, \tau) + \dots, \quad (3.5)$$

the left boundary condition in (2.10) yields

$$\partial\phi_i/\partial\xi = 0 \text{ at } \xi = 0; \quad i = 0, 1, 2, \dots$$

while the initial conditions

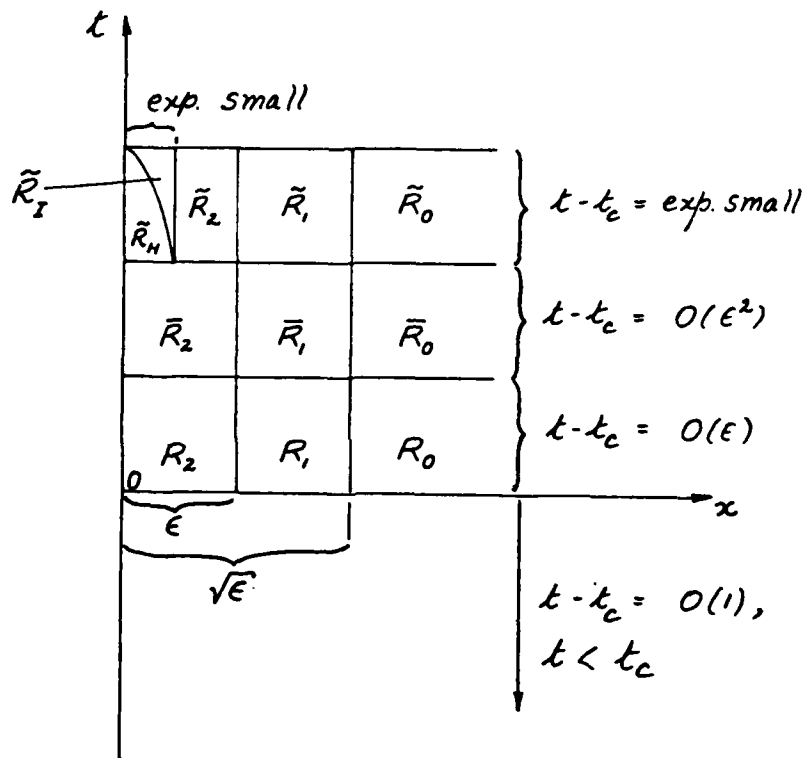


Figure 2. Various regions in the  $xt$ -plane (not to scale) from inert through explosion stages.

$$\phi_1(\xi, \infty) = 0$$

are a result of matching with the inert solution (3.1). The first two terms in (3.5) are found to be (see [11])

$$\phi_0 = f_0(\tau), \quad (3.6a)$$

$$\phi_1 = A_0(\xi + e^{-\xi})P(\tau) + f_1(\tau), \quad (3.6b)$$

where

$$P(\tau) = \exp[f_0(\tau) + (\pi t_0)^{-1/2} \tau], \quad (3.7)$$

and the yet unknown functions  $f_0, f_1$  satisfy

$$f_0(-\infty) = f_1(-\infty) = 0. \quad (3.8)$$

As  $\xi \rightarrow \infty$ , equations (3.6) show that  $\phi_0, \phi_1$  do not decay to zero, thereby violating the right boundary condition in (2.10). This suggests the presence of a new region  $R_1$ , separating  $R_2$  from the inert region  $R_0$ , as shown in Figure 2. In  $R_1$  the spatial coordinate is taken to be  $X$ , defined by

$$x = \sqrt{\epsilon} X \quad \text{or} \quad \xi = X/\sqrt{\epsilon}, \quad X > 0,$$

which reduces (2.9) to

$$\phi_\tau = \phi_{XX} + \sqrt{\epsilon} (A_0/R)(B - \phi) \exp[(\theta_C^2/\epsilon)(\theta_C^{-1} - (\theta_C - \sqrt{\epsilon} X + \xi + o(\sqrt{\epsilon}))^{-1})].$$

Anticipating  $\phi$  to be  $O(\epsilon)$ , it is clear that the reaction term in the above equation is exponentially small. On setting

$$\phi = \epsilon \psi_0(X, \tau) + \epsilon^{3/2} \psi_1(X, \tau) + \dots, \quad (3.9)$$

$\psi_0$  and  $\psi_1$  are found to satisfy

$$\left. \begin{aligned} \psi_{0\tau} &= \psi_{0XX}; \quad \tau > -\infty, \quad X > 0, \\ \psi_0(0, \tau) &= f_0(\tau), \quad \psi_{0X}(0, \tau) = -A_0 P(\tau), \quad \psi_0(\infty, \tau) = 0, \\ \psi_0(X, \infty) &= 0, \end{aligned} \right\} \quad (3.10)$$

and

$$\left. \begin{aligned} \psi_{1\tau} &= \psi_{1XX}; \quad \tau > -\infty, \quad X > 0, \\ \psi_1(0, \tau) &= f_1(\tau), \quad \psi_{1X}(0, \tau) = (3/2)A_0^2[P(\tau)]^2 - A_0 P(\tau) f_1(\tau), \quad \psi_1(\infty, \tau) = 0, \\ \psi_1(X, \infty) &= 0. \end{aligned} \right\} \quad (3.11)$$

The left boundary conditions\* in the two problems above result from matching with  $R_0$ , while the right boundary conditions and the initial conditions are provided by matching with the inert region  $R_0$ . Both the problems can be solved by using a Laplace transform in  $\eta$ . Thus, (3.10) has the transformed solution

$$\begin{aligned}\tilde{\psi}_0(x, \tau) &= \text{L.T. of } \psi_0(X, \tau) \\ &= \int_{-\infty}^{\tau} [-s f_0(\sigma) + A_0 \exp\{f_0(\sigma) + (\pi t_c)^{-1/2} \sigma\}] e^{s^2(\tau-\sigma)} d\sigma.\end{aligned}\quad (3.12)$$

An integral equation for the still-unknown function  $f_0(\tau)$  can be obtained by inverting  $\tilde{\psi}_0(s, \tau)$  and taking the limit  $\eta \rightarrow 0$ . It is convenient to write

$$f_0(\tau) = \bar{f}_0(\bar{\tau}), \quad (3.13)$$

where

$$\bar{\tau} = \ln[(\pi t_c)^{1/4} A_0] + (\pi t_c)^{-1/2} \tau. \quad (3.14)$$

Then  $\bar{f}_0$  satisfies the parameter-free integral equation

$$\bar{f}_0(\bar{\tau}) = (\pi)^{-1/2} \int_{-\infty}^{\bar{\tau}} (\bar{\tau} - \sigma)^{-1/2} \exp[\bar{f}_0(\sigma) + \sigma] d\sigma.$$

Liñán and Williams [11] obtain an equivalent integral equation, solve it numerically and show that  $\bar{f}_0$  is positive, monotone increasing and becomes unbounded at  $\bar{\tau} = h_0$ ; they find  $b_0$  to have the numerical value

$$h_0 = -0.431.$$

Following [11] we choose

$$A_0 = (\pi t_c)^{-1/4} e^{h_0} \quad (3.15)$$

which, through (3.13) and (3.14), places the singularity in  $f_0(\tau)$  at  $\tau = 0$ . The following asymptotic expansion can be developed:

\*Specification of  $\psi_1(0, \tau)$  in (3.11) requires carrying (3.5) to an additional term.



$$f_0(\tau) = -(1/2)\ln(-\tau) + \ln[\sqrt{\pi}/(2A_0)] + o(1) \text{ as } \tau \rightarrow 0^-. \quad (3.16)$$

(The above expansion also appears in [11] but there the second term seems to have a misprint.) Once  $f_0$  is known, (3.12) can be inverted to yield  $\psi_0(X, \tau)$ . We shall need the behavior of  $\psi_0(X, 0)$  for small  $X$ , and this can be calculated from the large  $s$  expansion of  $\tilde{\psi}_0(s, 0)$ . The result is

$$\psi_0(X, 0) = -\ln X + [\ln(\sqrt{\pi}/(2A_0))] - \gamma/2 + O(X^2) \text{ as } X \rightarrow 0, \quad (3.17)$$

where  $\gamma$  is the Euler's constant.

The unknown function  $f_1(\tau)$  can also be determined from (3.11) in an entirely analogous way, and is found to have the asymptotic behavior

$$f_1(\tau) = -(3/4)\pi^{3/2}(2 - \pi)^{-1}(-\tau)^{-1/2} + o(1) \text{ as } \tau \rightarrow 0^-.$$

Returning now to the region  $R_2$ , we note that the unboundedness of  $f_0$  and  $f_1$  leads to a breakdown of the expansion (3.5) as  $\tau \rightarrow 0^-$ . This is as far as Liñán and Williams [11] went; they identified the appearance of the singularity as thermal runaway, i.e. the onset of significant departures from the inert solution.

#### 4. IGNITION STAGE.

In order to continue the solution further in time, we observe that (3.5) yields

$$\phi_\tau \sim \frac{1}{2} \varepsilon (-\tau)^{-1} \text{ as } \tau \rightarrow 0,$$

indicating that the hitherto neglected unsteady term in (3.3) must be reinstated when  $\tau = O(\varepsilon)$ . This suggests a new time-variable  $T$ , defined via the scaling

$$\tau = \varepsilon T, \text{ or equivalently, } t = \varepsilon^2 T.$$

As Figure 2 indicates, the relevant regions in the  $xt$ -plane are  $\bar{R}_2$  (characterized by  $\xi$  and  $T$ ) and  $\bar{R}_1$  (characterized by  $x$  and  $T$ ). Of these, the latter is easily disposed of; in it (2.9) reduces to

$$\phi_T = \varepsilon \phi_{XX} + \text{est.}$$

Therefore, to leading order,  $\phi$  can depend only on  $x$ . Matching with  $R_1$  then gives

$$\phi = \varepsilon \psi_0(x, 0) + o(\varepsilon). \quad (4.1)$$

In  $\bar{R}_2$ , (2.9) assumes the form

$$\phi_T = \phi_{\xi\xi} + \varepsilon^{3/2} (A_0/B)(B - \phi) \exp[(\theta_c^2/\varepsilon)\{\theta_c^{-1} - (\theta_c + \phi - \varepsilon\xi + o(\varepsilon))^{-1}\}], \quad (4.2)$$

$$\xi > 0, \quad T > -\infty.$$

Matching with  $R_2$  as  $T \rightarrow -\infty$  dictates the expansion

$$\phi = -\frac{1}{2} \varepsilon \ln \varepsilon + \varepsilon [U_1(\xi, T) - \ln A_0] + \dots, \quad (4.3)$$

which, when substituted into (4.2), yields

$$U_{1T} = U_{1\xi\xi} + \exp(U_1 - \xi), \quad \xi > 0, \quad T > -\infty. \quad (4.4a)$$

The left boundary condition in (2.10) provides

$$U_{1\xi}(0, T) = 0 \quad (4.4b)$$

while matching with the  $\bar{R}_1$ -expansion (4.1) yields (cf. (3.17))

$$U_1 \rightarrow -\ln \xi + \left(\ln \frac{\sqrt{\pi}}{2} - \frac{1}{2} \gamma\right) \text{ as } \xi \rightarrow \infty. \quad (4.4c)$$

The initial condition

$$U_1 \sim -\frac{1}{2} \ln(-T) + \ln \frac{\sqrt{\pi}}{2} - \frac{2}{\sqrt{-\pi T}} v_0(\xi) \quad \text{as } T \rightarrow -\infty \quad (4.4a)$$

is the result of matching with the  $R_2$ -expansion (3.5). Here,

$$v_0(\xi) = \frac{3}{8} \pi^2 (2 - \pi)^{-1} + \frac{1}{4} \pi (\xi + e^{-\xi}) . \quad (4.5)$$

We observe first that the above problem for  $U_1$  is parameter-free, and therefore defines a universal function. Second, each of the three terms present in the full equation (2.9) still survives in the reduced form (4.4a), albeit the Arrhenius exponent has been simplified via linearization about a reference state (i.e. the inert state). This feature is reminiscent of the induction-period problem for self-induced combustion, discussed in [1], and we shall find that the similarity extends to the nature of the solution as well. Equations (4.4) were solved numerically by spacewise discretization, followed by a numerical integration of the resulting system of ordinary differential equations with the stiff ODE solver EPISODE B [17]. Prior to discretization, a coordinate transformation was used to map the problem onto a finite spatial domain.

The numerical solution is displayed in Figure 3. Initially the temperature rise is everywhere gradual, but then  $U_1$  begins to increase rapidly near  $\xi = 0$  while variations are more leisurely elsewhere. Eventually, at a definite time  $T_\infty (= -14.719)$ ,  $U_1(0, T)$  becomes unbounded. The evolution of the singularity at  $T_\infty$  can be examined analytically. (The following discussion will be brief, since the situation is analogous to that in [1].) We let

$$T = T_\infty - p, \quad p > 0, \quad (4.6)$$

and in the limit  $p \rightarrow 0$ , develop two asymptotic expansions for  $U_1$ . An outer expansion, valid away from  $\xi = 0$ , has the form

$$U_1 = U_{10}(\xi) + p U_{11}(\xi) + \dots, \quad (4.7)$$

where  $U_{10}(\xi)$  is the numerically computed solution of (4.4) at  $T = T_\infty$ , and the higher-order terms  $U_{1i}$  can be determined by substituting (4.7) into (4.4a). An inner region, or boundary layer, is characterized by the variables  $p$  and  $\eta$ , where

$$\eta = \xi/\sqrt{p}, \quad 0 < \eta < \infty, \quad (4.8)$$

and the inner expansion is seen to have the form

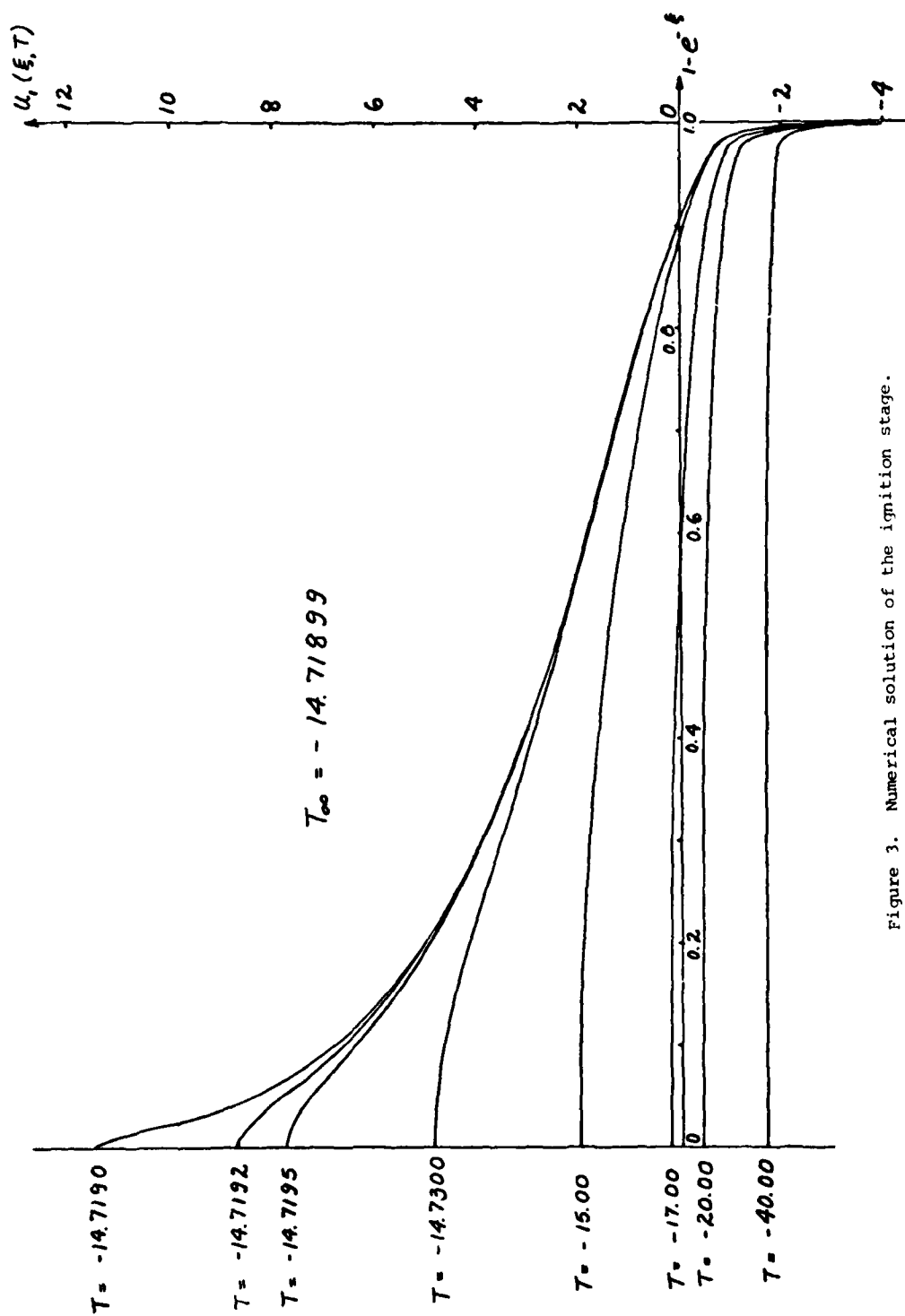


Figure 3. Numerical solution of the ignition stage.

$$U_1 = -\ln p + g_0(\eta) + \sqrt{p} g_1(\eta) + \dots \quad (4.8)$$

In the limit  $p \rightarrow 0$ ,  $\eta$  fixed, the boundary-layer thickness is  $O(\sqrt{T})$ , and the expansion (4.9) indicates explicitly that the singularity in  $U_1$  is logarithmic. When (4.9) is substituted into (4.4a), we obtain the following equation for  $g_0$ :

$$g_0'' - \frac{1}{2} \eta g_0' + \exp g_0 - 1 = 0, \quad 0 < \eta < \infty. \quad (4.10a)$$

The condition

$$g_0'(0) = 0 \quad (4.10b)$$

is by now familiar, while the behavior

$$g_0 = -2 \ln \eta + a_0 + O(\eta^{-2}) \quad \text{as } \eta \rightarrow \infty \quad (4.10c)$$

comes from suppressing the exponential growth of  $g_0$  for  $\eta \rightarrow \infty$ ; such a growth would not be commensurate with the slow rate of change observed outside the boundary layer. The constant  $a_0$  is determined by matching the expansions (4.7) and (4.9), which requires

$$U_{10}(\xi) = -2 \ln \xi + a_0 + O(\xi) \quad \text{as } \xi \rightarrow 0. \quad (4.11)$$

A comparison of the above asymptotic expression for  $U_{10}$  with the numerical solution of (4.4) at the edge of the boundary layer (i.e. for such a choice  $(\xi, T)$  which satisfies  $\xi \ll 1$ ,  $T_\infty - T \ll 1$  and  $\eta = \xi/\sqrt{T_\infty - T} \gg 1$ ) then yields  $a_0 (= 2.5)$ . With  $a_0$  known,  $g_0$  can be computed by integrating (4.10) backwards. The result is a monotonic curve with

$$g_0(0) > 0 \quad (4.12)$$

(see Figure 5 of [1]). The higher order  $g_1$  occurring in (4.9) can, in principle, be computed in an analogous way.

To summarize, we have shown that the ignition stage terminates at a definite time  $T_\infty$ . For  $T < T_\infty$ , the temperature increases throughout the  $O(\epsilon)$  thick surface layer  $\bar{R}_2$ , but remains an  $O(\epsilon \ln \epsilon)$  perturbation of the inert temperature (cf. (4.3)). Toward the end of the ignition period ( $T \rightarrow T_\infty$  or  $p \rightarrow 0$ ), a boundary layer, or hot spot, of thickness  $O(\sqrt{p} \epsilon)$  develops within  $\bar{R}_2$ . In the hot spot the solution grows rapidly and has the expansion

$$\phi = \frac{1}{2} \epsilon \ln \epsilon + \epsilon [-\ln p + g_0(\eta) - \ln A_0 + O(\sqrt{p})] + o(\epsilon), \quad \eta > 0, \quad (4.13)$$

while in the remainder of  $\bar{R}_2$  the solution remains

$$\phi = -\frac{1}{2} \epsilon \ln \epsilon + \epsilon [U_{10}(\xi) - \ln A_0 + O(p)] + o(\epsilon), \quad \xi > 0. \quad (4.14)$$

In the  $O(\sqrt{\epsilon})$  thick region  $\bar{R}_1$  the solution is constant in time, to leading order, during the entire ignition stage (cf. (4.1)) while in the inert region  $R_0$ ,  $\phi = 0$  to all algebraic orders in  $\epsilon$ .

As the process evolves further,  $O(1)$  departures from the inert solution will begin to occur at the surface. Therefore, it will be convenient to discard  $\phi$  in favor of  $\theta$  as the dependent temperature variable.

## 5. EXPLOSION STAGE.

As  $p \rightarrow 0$ , the  $O(\sqrt{p} \epsilon)$  hot spot diminishes in size but grows in intensity, eventually causing the expansion (4.12) to break down when  $\epsilon \ln p = O(1)$ . The further development of the solution therefore takes place on the exponentially short time scale  $\sigma$ , defined by

$$\sigma = -\epsilon \ln(\sqrt{\epsilon} A_0 p), \quad \sigma > 0 \quad \text{and} \quad O(1). \quad (5.1)$$

correspondingly,  $\xi$  is exponentially small, and in particular,

$$\epsilon \ln \xi^2 = O(1)$$

at the edge of the hot spot.

The analysis again proceeds as in [1] and only a brief description will be given here. In terms of the new hot spot variables  $\eta$  and  $\sigma$ , equation (2.9) reads

$$\theta_{\eta\eta} - \frac{1}{2} \eta \theta_{\eta} - \epsilon \theta_{\sigma} + (\epsilon/R)(B + \theta_I - \theta) \exp[(\theta_c^2/\epsilon)(\theta_c^2(\theta_c - \sigma) - \theta^{-1})] \quad (5.2)$$

where (2.8) has been employed to replace  $\phi$  by  $\theta$ . From (2.7) and (3.2) we note that in the hot spot,

$$\theta_I = \theta_c + \text{est.} \quad (5.3)$$

Also, the left boundary condition in (2.2a) reduces to

$$\partial\theta/\partial\eta = 0 + \text{est. at } \eta = 0, \quad (5.4)$$

i.e. the time scale of the explosion stage is so small that practically no heat enters the surface. It can then be shown that the solution of (5.3) satisfying (5.4) and matching with the ignition stage has the expansion

$$\theta = \theta_c^2(\theta_c - \sigma)^{-1} + \epsilon \theta_c^2(\theta_c - \sigma)^{-2} [g_0(\eta) - \ln \frac{(\theta_c - \sigma)^2 \{ \theta_c + B - \theta_c^2(\theta_c - \sigma)^{-1} \}}{R \theta_c^2}] + \dots \quad (5.5)$$

Here  $g_0(\eta)$  is the same function that appeared in (4.9), i.e. the hot spot retains the spatial structure that it possessed at birth.

Outside the hot spot (denoted by  $\bar{R}_H$  in Figure 1), i.e. for  $\xi = O(1)$  and beyond, the solution remains essentially frozen at its state at the end of the ignition stage. This is because these diffusion-dominated regions are unable to respond to exponentially rapid variations. Thus, in the inert region  $\bar{R}_0$ , the solution is

$$\theta = \theta_I(x, t) = \theta_I(x, t_c + \epsilon^2 T_\infty) + \text{est} \quad (5.6)$$

while in  $\tilde{R}_1$  and  $\tilde{R}_2$  the solution is, respectively,

$$\theta = \theta_I(\sqrt{\epsilon} X, t_c + \epsilon^2 T_\infty) + \epsilon \psi_0(X, 0) + o(\epsilon) \quad (5.7)$$

and

$$\theta = \theta_I(\epsilon \xi, t_c + \epsilon^2 T_\infty) - \frac{1}{2} \epsilon \ln \epsilon + \epsilon [U_{10}(\xi) - \ln A_0] + o(\epsilon). \quad (5.8)$$

The last two expressions follow from (4.1) and (4.13), respectively, in conjunction with the relation  $\theta = \theta_I + \phi$ .

The hot-spot solution (5.5) does not match with the  $\tilde{R}_2$ -solution (5.8). As pointed out in [1], this is due to the logarithmic behavior of  $U_{10}(\xi)$  for  $\xi \rightarrow 0$  (cf. (4.7)), which causes (5.8) to break down before the edge of  $\tilde{R}_H$  is reached. The situation is remedied by recognizing that an intermediate region  $\tilde{R}_I$  has now evolved (see Figure 1), separating the rapidly shrinking  $\tilde{R}_H$  from  $\tilde{R}_1$ , and characterized by the variables  $\sigma$  and  $z$ , where

$$z = -\epsilon \ln(\sqrt{\epsilon} A_0 \xi^2), \quad 0 < z < \sigma. \quad (5.9)$$

By rewriting (2.9) in terms of the new variables, it can be shown that the intermediate expansion proceeds as

$$\theta = \theta_c^2 (\theta_c - z)^{-1} + \epsilon \theta_c^2 (\theta_c - z)^{-2} [a_0 - \ln \frac{(\theta_c - z)^2 \{ \theta_c + R - \theta_c^2 (\theta_c - z)^{-1} \}}{R \theta_c^2}] + \dots, \quad (5.10)$$

which matches with the outer solution (5.8) as  $z \rightarrow 0$  and with the hot spot solution (5.5) as  $z \rightarrow \sigma$ . This completes the description of the explosion stage.



## 6. DETACHMENT STAGE

The hot spot reaches maturity at  $\sigma = B\theta_c/(\theta_c + B)$ . Then, as shown in Figure 1,  $\sigma$  approaches its maximum value  $\theta_c + B$  and the mass fraction of the reactant,  $Y$ , falls to zero inside the hot spot. At the same time, a logarithmic singularity develops in the second term of the hot-spot solution (5.5), signalling a breakdown, while the expansions (5.6-5.8) and (5.10), pertaining to regions outside the hot spot, still hold. Further evolution of the hot spot is now governed by the independent variables  $\chi$  and  $s$ , where

$$x = \delta\chi \quad \text{and} \quad t = t_c + \epsilon^2 T_\infty + \delta^2 s,$$

and the exponentially small parameter  $\delta$  is defined by

$$\delta^2 = (B/A_0)\epsilon^{1/2} \exp[-B\theta_c/(2\epsilon(\theta_c + B))].$$

Since the above scaling implies

$$\sigma = B\theta_c/(\theta_c + B) - \epsilon \ln(-Bs/\epsilon),$$

we expect the detachment stage to match with the explosion stage as  $s \rightarrow -\infty$ . In the new variables, (2.9) reads

$$\theta_s = \theta_{\chi\chi} + (\theta_c + B - \theta + \epsilon s t) \exp[(\theta_c^2/\epsilon)\{(\theta_c + B)^{-1} - \theta^{-1}\}],$$

which suggests the following expansion:

$$\theta = \theta_c + B + \epsilon w_1(\chi, s) + \dots, \quad (6.1)$$

where

$$\epsilon = (\theta_c + B)^2 \epsilon / \theta_c^2.$$

The problem for  $w_1$  is found to be

$$w_{1s} = w_{1\chi\chi} - w_1 e^{w_1}, \quad \chi > 0, \quad s > -\infty, \quad (6.2a)$$

$$w_{1\chi}(0, s) = 0, \quad (6.2b)$$

$$w_1 \rightarrow -\ln \chi^2 - \ln(\ln \chi^2) + a_0 \quad \text{as } \chi \rightarrow \infty, \quad (6.2c)$$

$$w_1 \rightarrow -\ln(-s) - \ln\{\ln(-s)\} + g_0(\chi/\sqrt{-s}) \quad \text{as } s \rightarrow -\infty, \quad \chi/\sqrt{-s} \text{ fixed}. \quad (6.2d)$$

The argument behind the left boundary condition (6.2b) is the same as that behind (5.4).

analogous to those for the transition-stage problem encountered in [1], and were solved by a similar numerical procedure. The solution, displayed in Figure 4, exhibits an expanding region adjacent to the surface in which  $w_1$  approaches zero as  $s$  increases. At the same time the region of significant spatial structure is pushed farther and farther into the interior. Thus, as the last remnants of the reactant are consumed, the hot spot evolves into a travelling front, or flame, or deflagration wave.

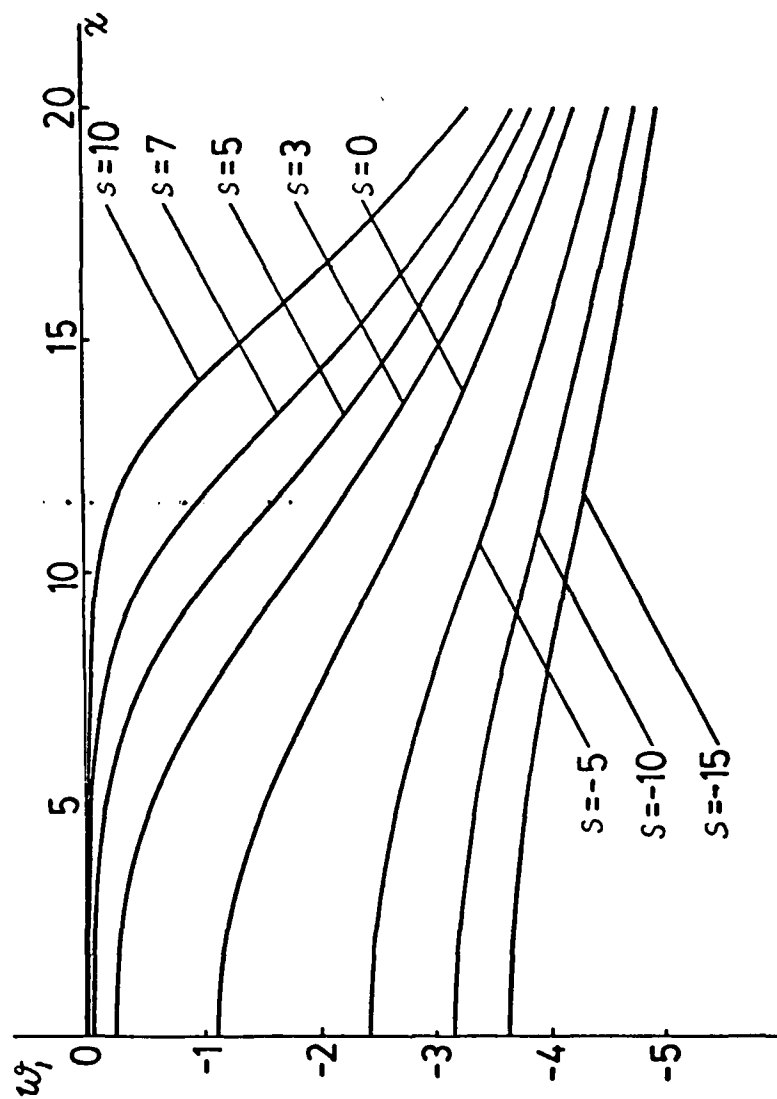


Figure 4. Numerical solution of the detachment stage.

## 7. PROPAGATION STAGE

In this section the speed and structure of the propagating wave are determined. The structure is found to be quasi-steady and self-similar (see Figures 1 and 5). It consists of a thin reaction zone surrounded by a slightly thicker envelope which separates the cold material ahead of the front from the burnt material behind (cf. [1]). The portion of the envelope ahead of the reaction zone is a preheat region where the material is brought up to the reacting temperature.

Figure 1 shows that the temperature of the cold material into which the front advances falls steadily away from the surface. This leads to a gradual retardation and thickening of the flame, as we shall see. Let  $x_0$ , taken to be  $O(1)$ , be the time-varying location of the flame. We shift to a reference frame in which the flame is at rest by setting

$$x = x_0 + (\delta_1/\epsilon_1)\zeta, \quad (7.1)$$

where  $\zeta$  is the spatial coordinate in the envelope. The small parameters  $\delta_1$  (exponentially small in  $\epsilon$ ) and  $\epsilon_1$  (proportional to  $\epsilon$ ), themselves dependent upon  $x_0$ , are to be assigned. The scaling (7.1) clearly implies that  $\delta_1/\epsilon_1$  is the thickness of the envelope. We shall later find that  $\delta_1$  is the thickness of the reaction zone within the envelope. The appropriate time scale  $\tau$  for the propagation stage is defined via the expression

$$t = t_c + \epsilon^2 T_\infty + (\delta_1/\epsilon_1)\tau, \quad \tau > 0, \quad (7.2)$$

indicating that the solution continues to evolve with exponential rapidity. The wave speed now emerges as

$$\frac{dx_0}{dt} = \frac{\epsilon_1}{\delta_1} \frac{dx_0}{d\tau} = \frac{\epsilon_1}{\delta_1} U(\tau), \quad (7.3)$$

say, where  $U(\tau)$  is  $O(1)$ . The inert temperature at  $x_0$  will play a critical role; therefore we set

$$\theta_I^0 = \theta_I(x_0, t_c + \epsilon^2 T_\infty) \quad (7.4)$$

and observe, from (2.7) and (7.2), that for  $\tau = O(1)$ ,

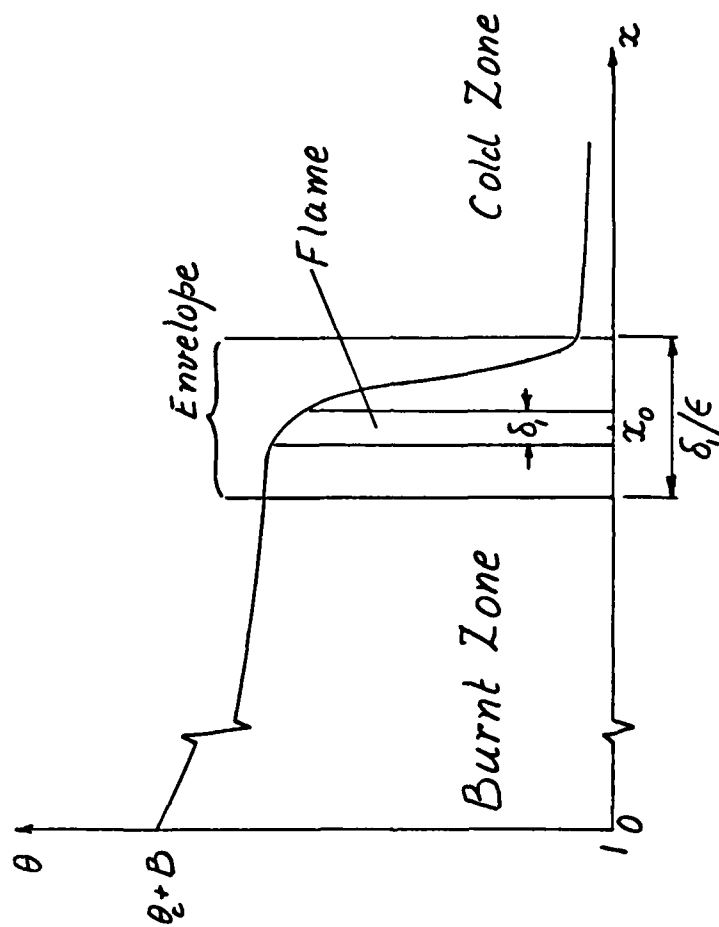


Figure 5. Propagation-stage profile.

$$\theta_I(x_0, t) = \theta_I^0 + \text{est} . \quad (7.5)$$

We can now define  $\delta_1$  and  $\epsilon_1$  as follows:

$$\delta_1^2 = (B/A_0) \epsilon^{1/2} \exp[(\theta_C^2/\epsilon) \{(\theta_I^0 + B)^{-1} - \theta_C^{-1}\}] \quad (7.6a)$$

and

$$\epsilon_1 = (\theta_I^0 + B)^2/E = (\theta_I^0 + B)^2 \epsilon / \theta_C^2 . \quad (7.6b)$$

Thus, both  $\delta_1$  and  $\epsilon_1$  depend upon  $x_0$  through  $\theta_I^0$ . Since  $\theta_I^0$  decreases monotonically (to unity) as  $x_0$  increases (cf. (2.7) and (7.4); also see Figure 1),  $\delta_1$  increases while  $\epsilon_1$  decreases with  $x_0$ . However, the ratio  $\delta_1/\epsilon_1$  increases, so that as the flame advances it thickens and, from (7.3), its speed falls.

In the  $\zeta, r$  variables, (2.9) transforms into

$$\begin{aligned} \delta_1 [\epsilon_1 - r U (\partial \theta_I^0 / \partial x_0)] \theta_r &= \theta_{\zeta \zeta} + U \theta_{\zeta} + \\ \epsilon_1^{-2} (\theta_I + B - \theta) \exp[(\theta_I^0 + B)^2/\epsilon] \{(\theta_I^0 + B)^{-1} - \theta^{-1}\} &, \quad (7.7) \\ -\infty < \zeta < \infty, r > 0 . \end{aligned}$$

The subsequent analysis follows along the lines of that in section 6 of [1], so that a brief account should suffice. Separate solutions need to be constructed for the reaction zone, the envelope and the region outside the front. In this outer region (see Figure 1),

$$\theta = \begin{cases} \theta_I(x, t) + B = \theta_I(x, t_C + \epsilon^2 T_\infty) + B + \text{est}, x_0 < 0 \text{ (burnt region)} , & (7.8a) \\ \theta_I(x, t) = \theta_I(x, t_C + \epsilon^2 T_\infty) + \text{est}, x_0 > 0 \text{ (cold region)} . & (7.8b) \end{cases}$$

The burnt-region solution (7.8a) is an exact solution of (7.8), satisfying the surface boundary condition in (2.2a), while the cold-region solution (7.8b) is just the frozen solution (5.6). In the envelope the portion  $\xi < 0$  is a part of the burnt region, i.e.

$$\theta = \theta_I^0 + B + \text{est}, \xi < 0 . \quad (7.9a)$$

For  $\xi > 0$ , chemistry is still unimportant since  $\theta < \theta_I^0 + B$ . The leading-order balance in (7.7) is therefore diffusive-convective, yielding

$$\theta = A_1(s) + B_1(s) \exp[-U(s)\xi] + \dots . \quad (7.9b)$$

Continuity of (7.9a,b) across  $\xi = 0$  gives

$$A_1 + R_1 = \theta_I^0 + P \quad (7.10)$$

while matching between the preheat solution (7.9b) and the cold-region solution (7.9b) leads to

$$A_1 = \theta_I^0. \quad (7.11)$$

Then, (7.10) determines  $B_1$ , i.e.

$$R_1 = B. \quad (7.12)$$

The remaining unknown  $U$  is determined by analyzing the structure of the reaction zone.

This is accomplished by the reaction-zone scaling

$$\xi = \epsilon_1 \rho$$

(which confirms that  $\delta_1$  is the thickness of the reaction zone) and the reaction-zone expansion

$$\theta = \theta_I^0 + B + \epsilon_1 v(\rho, r) + \dots,$$

which reduce (7.7), to leading order, to

$$v_{\rho\rho} - v \exp v = 0, \quad -\infty < \rho < \infty. \quad (7.13)$$

Matching with (7.9a,b) provides the boundary conditions

$$v \rightarrow 0 \text{ as } \rho \rightarrow -\infty, \quad v \rightarrow -B_1 U \text{ as } \rho \rightarrow \infty$$

which, when applied to the first integral of (7.13), yield

$$B_1 U = \sqrt{2}$$

whence (7.12) leads to

$$U(s) = \sqrt{2}/B. \quad (7.14)$$

On substituting for  $U$ ,  $\epsilon_1$  and  $\delta_1$  in (7.3), the speed of the flame is seen to be

$$\frac{dx_0}{dt} = \frac{(\theta_I^0 + B)^2}{\theta_c^2} \sqrt{\frac{2A_0 \epsilon}{B^3}} \exp \left[ \frac{\theta_c^2}{2\epsilon} \left\{ -\frac{1}{\theta_I^0 + B} + \frac{1}{\theta_c} \right\} \right]. \quad (7.15)$$

The ultimate, steady flame speed will correspond to  $\theta_I^0 = 1$  in the above expression; the right inequality of (2.5) guarantees that this speed will not be exponentially small.

The above analysis is predicated upon  $x_0$  being  $O(1)$ , which leads to the temperature immediately ahead of the flame being essentially due to inert heating. Such is

not the case when the flame is very close to the surface. Let  $x_0$  be exponentially small, i.e. let

$$x_0^2 = (\varepsilon^{3/2}/A_0)e^{-z_0/\varepsilon}, \quad 0 < z_0 < R\theta_c/(\theta_c + B).$$

Then, the front edge of the flame lies in the intermediate region discussed in section 5, and there the temperature differs from the inert solution by an  $O(1)$  amount (cf. (5.10)). It can be shown that (7.14) must then be replaced by

$$U(s) = \sqrt{2}/[\theta_c + B - \theta_c^2(\theta_c - z_0)].$$

As  $z_0 \rightarrow 0$ , (7.14) is recovered. As  $z_0 \rightarrow R\theta_c/(\theta_c + B)$ ,  $U$  becomes singular, suggesting a breakdown of the analysis. This is to be expected, because the flame, at that time, is still in the detachment stage discussed earlier.



#### 8. CONCLUDING REMARKS

An asymptotic description of the evolution of a deflagration wave in an initially solid material under the stimulus of a constant heat flux has been given. The analysis reveals that the situation is quite similar to that for self-induced combustion, discussed earlier [1], with the exception that the thermal explosion process responsible for the birth of the hot spot is now confined to a thin surface layer. Furthermore, it is found that once ignition has occurred, events evolve so rapidly that the system becomes oblivious to the presence of the external heat supply.

To be sure, the results are based upon the assumption of the Lewis number being unity. However, the case  $L = \infty$ , corresponding to solid combustibles, was also analyzed. The full system (2.1-2.3) must then be dealt with head on, since (2.6) no longer obtains. The reactant equation (2.1b) does simplify due to the absence of the diffusion term, and the boundary conditions (2.2b) have to be abandoned. Otherwise, the analysis proceeds in an analogous way. Up to the end of the explosion period, such calculations for the case of self-induced combustion appear in the forthcoming paper by Kassoy and Poland [3].

The results differ from the  $L = 1$  case only in one significant respect. As long as combustion is confined to a stationary zone adjacent to the surface (i.e. prior to the detachment of the hot spot), any reactant consumed there is not replenished by diffusion from outside. Therefore, for a given temperature rise, the reactant concentration falls to a lower value within the zone than it would if diffusion of reactant were permitted. This effect appears as early as the transient stage. Thus, Linán and Williams [11] found that an  $O(\epsilon)$  change in  $\phi$  corresponds to a (much larger)  $O(\sqrt{\epsilon})$  change in  $Y$ . The same holds true during the ignition period. By the time the explosion stage ends, it is seen [3] that the maximum temperature reached in the stationary hot spot is lower, by as much as an  $O(1)$  amount, than the corresponding value for the case  $L = 1$ . The propagating flame does not suffer from such a fate because it obtains the necessary reactant supply through convection.

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